FINAL PROJECT OF QUANTUM MECHANIC COURSE DURING FALL 2021: APPLICATION OF BOOTSTRAP METHOD TO QUANTUM MECHANICAL SYSTEMS

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In this report, a brief introduction to the principle of the Bootstrap method applied to one dimensional quantum mechanical system is given. The results and analysis of the application to the spinless electron in Hydrogen atom is demonstrated. Also, the methods of application to other potentials is derived.

I. INTRODUCTION

Recently, as inspired by the Bootstrap method used in conformal field theory [1], the application of Bootstrap method to one dimensional quantum mechanical system paves a new path toward calculating the energy spectrum of such systems. Through this method, one calculate the energy spectrum by using only the information about the observables. Besides, there exist an exact limit for this method to obtain the definite energy spectrum.

In this report, I briefly introduce the principle of this method in section II. Then, I analyze the application of this method to calculate the spectrum of spinless electron in Hydrogen atom in section III. Further, I also derived the methods for application to other potentials in section IV. Eventually, a summary about this report and the comments about the Bootstrap method applied to quantum mechanical system is given in section V.

II. INTRODUCTION TO THE THEORY

A. General Theory

The basic ideas of the Bootstrap method is to relate series of observables to each other and the eigenenergies through some recursion relations. Then, by using the constraints that will be mentioned later, one can find the eigenergies through scanning the energy spectrum.

More specifically, the Bootstrap method relies on the following three obvious properties:

$$\langle [H, O] \rangle = 0 \tag{1}$$

and

$$\langle HO \rangle = E \langle O \rangle \tag{2}$$

and

$$\langle O^\dagger O \rangle \geq 0 \tag{3}$$

, where $\langle ... \rangle$ uses an energy eigenstate as basis and E is the corresponding eigenenergy; H is the Hamiltonian of the system and O is an arbitrary operator.

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If we expand the operator O into polynomials of the **moment** $M = M(x, p)$, which is a function of position operator x and momentum operator p :

$$O = \sum_s a_s M^s \tag{4}$$

Then, equation (1.) will generate a recursion relation which relates the $\langle M^s \rangle$ with different s to each other. With the aid from equation (2.), the $\langle M^s \rangle$ for most of the s can be related to the eigenenergy E. Eventually, equation (3) will gives the constraint that **the moment matrix** m with its matrix elements giving by:

$$(m)^{ij} = \langle M^{*i} M^j \rangle \tag{5}$$

should be semi-positive definite since the a^s in equation (4.) is arbitrary.

Because **the principle minors of a semi-positive matrix are also semi-positive**, one can impose this constraints to the matrix in equation (5.) to obtained the allowed range for the eigenergies E. Note that, in the above steps only the information about observables are needed, which differs from the usual textbook formalism such as Schrodinger's wave mechanic.

B. A Particle Subject to an Arbitrary Non-Periodic Potential

In the case when the Hamiltonian is (in atomic unit):

$$H = \frac{p^2}{2} + V(s) \tag{6}$$

,two moments M are used:

$$\begin{cases} M^s = x^s \\ M^s = x^s p \end{cases} \tag{7}$$

Then, equation (1) would gives:

$$\begin{cases} 0 = -s\langle x^{s-1} p \rangle + \frac{i}{2} s(s-1) \langle x^{s-2} \rangle \\ 0 = s\langle x^{s-1} p^2 \rangle + \frac{1}{4} s(s-1)(s-2) \langle x^{s-3} \rangle - \langle x^s V'(x) \rangle \end{cases} \tag{8}$$

and equation (2) would gives:

$$0 = E\langle x^s\rangle - \frac{1}{2}\langle x^s p^2\rangle - \langle x^s V(x)\rangle \tag{9}$$

for the first moment in equation (7.). Combine equation (8.) and equation (9.), one would have:

$$\begin{aligned}\langle x^s\rangle = \frac{-1}{8(s+1)E}[&(s+1)s(s-1)\langle x^{s-2}\rangle \\ &- \langle x^{s+1}V'(x)\rangle - 2(s+1)\langle x^s V(x)\rangle]\end{aligned} \tag{10}$$

, where the range of s would be determined by the explicit form of the potential $V(x)$.

III. APPLICATIONS TO SPINLESS ELECTRON IN HYDROGEN ATOM

For the spinless electron in Hydrogen atom, one can regard the radial part of the Hamiltonian as the one dimensional quantum mechanical system to be discussed. The potential is thus:

$$V(r) = \frac{l(l+1)}{2r^2} - \frac{1}{r} \tag{11}$$

, where l is the orbital angular momentum. Equation 10. therefore becomes:

$$\begin{aligned}\langle r^s\rangle = \frac{-1}{8(s+1)E}[&s((s+1)(s-1) - 4l(l+1))\langle r^{s-2}\rangle \\ &+ 4(2s+1)\langle r^{s-1}\rangle]\end{aligned} \tag{12}$$

, where $s \geq 0$ is required[1]. Since one can obtain the relation $\langle r^{-1}\rangle = -2E$ when $s = 0$ and the fact that $\langle r^s\rangle, s < -1$ does not appear when $s \geq 1$, one just need to scan the energy E to find the allowed eigenenergy.

Besides, since $\langle r^s\rangle$ have a factorial growth when s is large, one can rescale the moment matrix element constructed through equation (5.) by: [1]

$$\frac{(m)^{ij}}{(m)^{i1}(m)^{j1}} \tag{13}$$

to reduce the numerical precision needed, of which the semi-positive definiteness is preserved.

A. The Algorithm

The procedure of the computation goes like:

1. For a given l at a given energy E, first generate $\langle r^s\rangle$ through equation (12.) from $s = 0$ to $s = 2(k-1)$, where k is the size of the moment matrix.
2. Construct the moment matrix through equation (5.) by using the results from the last step.
3. Rescale the moment matrix through equation (13.)
4. Check the semi-positive definiteness for all the principle minor of the moment matrix through checking the sign of their determinant.
5. Once a principle minor appears a negative sign for its determinant, the sign checks for the rest principle minors at this energy level are skipped. The sign of the determinant of the skipped principle minors are set to be 0.
6. Record the sign of all the principle minors at all energy level within a desired energy window to proceed the analysis.

The above algorithm is implemented through *Matlab* [2] to generate the results in next section.

B. Implementation Results

The calculation are proceed with:

1. numerical precision of 32 digits
2. energy window $E \in [-0.15, 0]$ ($E \in [-0.51, -0.49]$ for scanning of ground state)
3. scanning step $dE = 10^{-5}$
4. orbital angular momentum l from 0 to 4
5. moment matrix with size K being 30×30

Figure (1.) to figure (6.) demonstrate the scanning results for different angular momentum l from 0 to 4, respectively. The energy of the n^{th} level in the spinless electron in Hydrogen atom is (in atomic unit):

$$E_n = \frac{1}{2n^2} \tag{14}$$

, which is marked as vertical solid lines for $n = 1$ to $n = 8$ in these figures. In this figures,

C. Analysis

The most anomalous results is that the ground state of the spinless electron in Hydrogen can be scanned by Bootstrap method as shown in figure (1.), which differ from the results in ref.[1]. Besides, the $l = 0$ results as shown in figure (2.) are actually scanned successfully, too. The difficulty mentioned in ref. [1] never occurred.

[1] Otherwise, one would need the information about $\langle r^\infty\rangle$ for $\langle r^s\rangle$ with $s < -1$

[2] The source codes can be found on my github page: `https://github.com/lengentyh/BootstrappedQM`

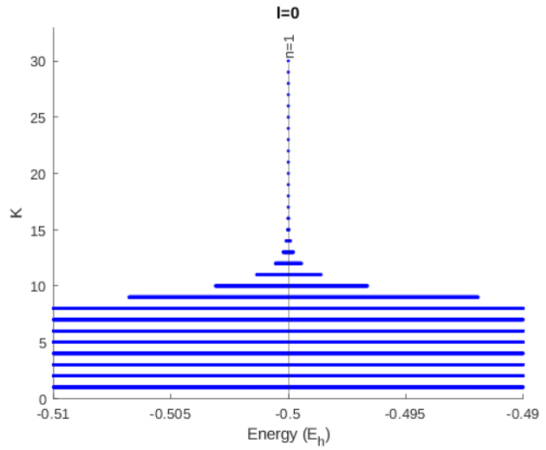

FIG. 1. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 0$

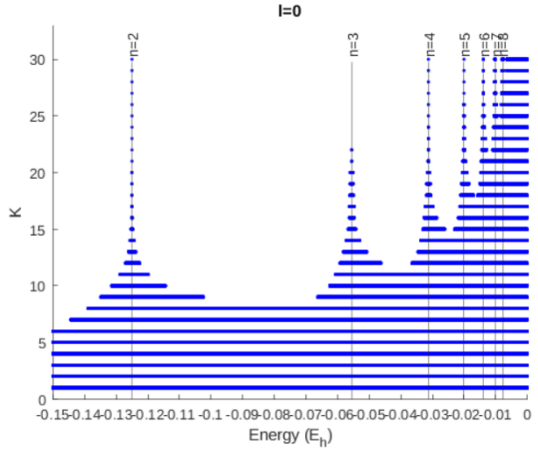

FIG. 2. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 0$

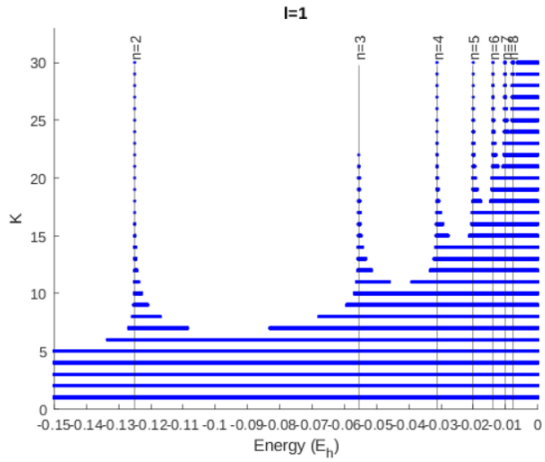

FIG. 3. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 1$

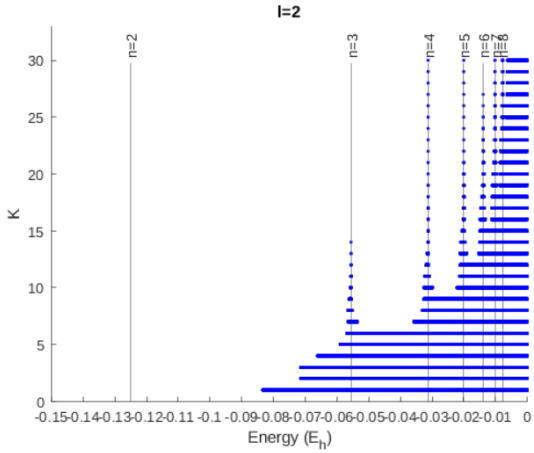

FIG. 4. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 2$

Overall speaking, the allowed energy ranges seems to converge more quickly from the left than the right in all the figures (except figure (1.)) as the size of the moment matrix K increase. And the convergence speed is so quick that the $n = 3$ level, which has an irrational energy value, cannot be scanned by the step with $dE = 10^{-5}$ for large enough K. Meanwhile, only as K increase, the higher energy levels can be scanned. Therefore, the size of K affect not only the convergence of the allowed energy ranges, but also the number of energy levels can be scanned. As analyzed in the beginning of section III, high numerical precision thus needed for both the highly-converged allowed energy ranges and the presence of high energy levels in the scanning results.

Further, the allowed energy ranges converge faster as the value of orbital angular momentum l increase. The example is the $n = 6$ level, which also has an irrational energy value and can be scanned by $l = 0$ and $l = 1$ when $K = 30$. However, as $l \geq 2$, the allowed energy range around this level converge so fast that it can no longer be scanned by the step with $dE = 10^{-5}$ when $K = 30$. Same things happened for the $n = 7$ level as $l \geq 3$. This fact can also be seen by observing the width of allowed energy range directly from the figures.

IV. OTHER APPLICATIONS

A. Inclusion of Spin-Orbit Coupling

When the spin-orbit coupling:[2]

$$V_{so}(r) \simeq \frac{1}{r^3}[j(j+1) - l(l+1) - s(s+1)]\frac{1}{16\pi \cdot 137^2} \quad (15)$$

is included, equation (12.) would have an additional term:

$$(2s-1)\langle r^{s-3}\rangle A(j,l,s) \quad (16)$$

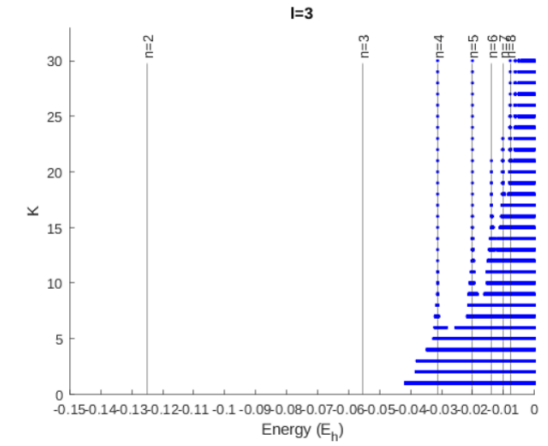

FIG. 5. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 3$

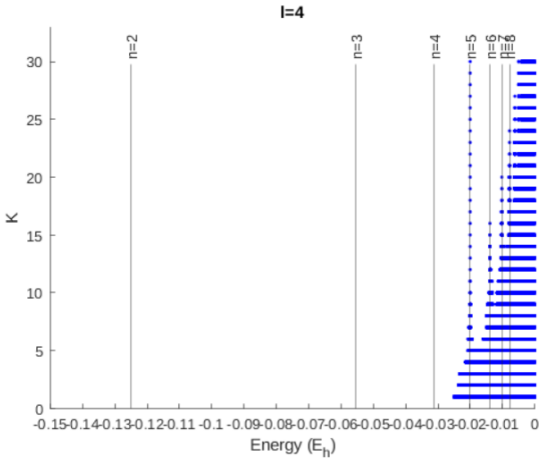

FIG. 6. Evolution of allowed energy ranges as the size of the moment matrix K increase for $l = 4$

,where $A(j,l,s) = \frac{[j(j+1)-l(l+1)-s(s+1)]}{16\pi\cdot 137^2}$. Still, $s \geq 0$ is required. When $s = 0$, one would obtain the relation:

$$1 = -\frac{\langle r^{-1}\rangle}{2E} - A(j,l,s)\langle r^{-3}\rangle \tag{17}$$

Meanwhile, when $s = 1$, one would obtain the relation:

$$\langle r\rangle = -\frac{1}{16}(-4l(l+1)\langle r^{-1}\rangle + 12) + A(j,l,s)\langle r^{-2}\rangle \tag{18}$$

Therefore, one not only need to scan the energy E, but also need to scan the value of $\langle r^{-2}\rangle$ and $\langle r^{-3}\rangle$ to find the allowed eigenenergies.

B. Application to Periodic Potential

When the potential is periodic in space, for example:

$$H = \frac{p^2}{2} + cos(kx), \text{for some k is real} \tag{19}$$

,one should better choose the moments M be:

$$\begin{cases} M^s = e^{iskx} \\ M^s = e^{iskx}p \end{cases} \tag{20}$$

Then, equation (1.) would give:

$$\begin{cases} 0 = sk\langle e^{iskx}p\rangle + \frac{(sk)^2}{2}\langle e^{iskx}\rangle \\ 0 = sk\langle e^{iskx}p^2\rangle + \frac{(sk)^2}{2}\langle e^{iskx}p\rangle - i\cdot k\cdot\langle sin(kx)e^{iskx}\rangle \end{cases} \tag{21}$$

and equation (2.) for the first moment in equation (20.) would give:

$$\langle e^{iskx}\frac{p^2}{2}\rangle + \frac{1}{2}(\langle e^{i(k+sk)x}\rangle + \langle e^{-i(k-sk)x}\rangle) = E\langle e^{iskx}\rangle \tag{22}$$

Therefore, combine equation (21.) and equation (22), one would get:

$$\begin{aligned}\langle (e^{ikx})^{s+1}\rangle = \frac{1}{s+\frac{1}{2}}[s(2E - \frac{s^2}{4}k^2)\langle (e^{ikx})^s\rangle \\ - (s-\frac{1}{2})\langle (e^{ikx})^{n-1}\rangle]\end{aligned} \tag{23}$$

, where $s \geq 0$ is required. Since when $s = 0$, one would obtain the relation:

$$\langle e^{ikx}\rangle = \langle (e^{ikx})^{-1}\rangle \tag{24}$$

, one would need to scan the energy E and the value of $\langle e^{ikx}\rangle$ to find the allowed eigenenergies. Fortunately, since the 2×2 matrix of equation (5.) for the first moment in equation (20.) is:

$$\begin{pmatrix} 1 & \langle e^{ikx}\rangle \\ \langle (e^{ikx})^{-1}\rangle & 1 \end{pmatrix} \tag{25}$$

, one would obtain $\langle e^{ikx}\rangle \in [-1,1]$ due to the constraint of semi-positive definiteness.[3]

V. SUMMARY AND COMMENTS

In this report, a brief introduction to the principle of the Bootstrap method applied to one dimensional quantum mechanical system is given. Also, the recursion relation of the moment for arbitrary potentials (including periodic potentials) are derived. The Bootstrap method is applied to the radial part of the spinless electron in Hydrogen atom to find the energy levels through *Matlab*. Then, the implementation results and the effect of including spin-orbit coupling are discussed.

The Bootstrap method indeed paves a new way toward finding the energy spectrum of a one dimensional system. However, the ability of generalize this method to higher dimension or interacting many-body systems is doubt. Although this method can have very fine resolution for

the energy spectrum, it also have the difficulty of finding higher energy levels as previous methods due to the factorial growth of the moment. Beside, the required high numerical precision and the scanning process also make the computation time consuming.

A better way of using the Bootstrap method to a one dimensional quantum mechanical system should be using other (approximate) methods to obtain rough ranges of the energy levels first, then apply the Bootstrap method within these ranges for precise values of the energy levels. Also, one can optimize the mesh (e.g. use adaptive mesh) used for the scanning process to accelerate the computation.

[1] D. Berenstein and G. Hulsey, Bootstrapping simple qm systems (2021), arXiv:2108.08757 [hep-th].
[2] D. J. Griffiths and D. F. Schroeter, *Introduction to Quantum Mechanics*, 3rd ed. (Cambridge University Press, 2018) Chap. 8.
[3] D. Berenstein and G. Hulsey, Bootstrapping more qm systems (2021), arXiv:2109.06251 [hep-th].